Proceedings of SPIE - The International Society for Optical Engineering, 1996, vol.2706, pages 193-200

Theory of isotopic effects in the optical spectra of lanthanide ions in crystals

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Abstract

Physical mechanisms contributing to the isotopic structure of spectra of the insulating activated crystals induced by the isotopic disorder in the host crystal or in a system of the impurity optical centers is considered. The microscopic theory of the geometrical anharmonic isotopic effect is presented. We show that the local deformation due to a mass defect in the crystal lattice is dominant in the formation of the fine specific spectral structure in crystals with the proper inhomogeneous isotopic composition (such as 6Li c 7Li 1-cYF 4:Ho with the natural abundance of c equals 7.42% of the 6Li isotope). It contributes essentially to the observed shifts of the spectral lines in the case of different masses of the active optical centers (such as 164Er, 166Er, 168Er and 170Er isotopes in the LiYF 4 crystal) as well. Detailed calculations of crystal field parameters and of their first and second derivatives with respect to the lattice strains for the impurity lanthanide ions in lithium-yttrium double fluorides are performed within the framework of the exchange charge model and used in the estimations of the different contributions to the isotope-induced shifts of the Stark sublevels.